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AFRL-SR-AR-TR-03-

0270

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1. REPORT DATE (DD-MM-YYYY)
3-7-2003

2. REPORT TYPE
Final Technical

3. DATES COVERED (From - To)
15-4-2000 - 14-4-2003

4. TITLE AND SUBTITLE

THEORETICAL STUDIES OF THE SENSITIVITY OF ENERGETIC MATERIALS

5a. CONTRACT NUMBER

5b. GRANT NUMBER
F49620-00-1-0273

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Oklahoma State Univerisity
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Office of
Scientific Research

20030731 058

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approve for Public Release: Distribution Unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The research supported by AFOSR grant F49620-00-1-0273 for the period 15 April 2000 to 14 April 2003 is described. The purpose of this research program is to develop atomic-level models for high energy density materials (HEDM), and to study their fundamental properties and behaviors that determine their suitability as practical propellants and explosives. The central focus of our research during this grant period was ionic energetic materials, although some studies of the interactions and reactions of energetic molecules with solid Al and Al_2O_3 , and of the hydrogen-bonded energetic solid 1,1-diamino-2,2-dinitroethylene (FOX-7) were performed. The primary purpose of the work was to develop accurate models for describing the physical properties of strong oxidizing salts. We have successfully modeled crystal structures, melting, and liquid properties of ammonium dinitramide as a test case for our approaches, and we have partially developed models for ammonium nitrate and hydroxylammonium nitrate. A long-term goal of this work is to model the chemistry of ionic liquids and thus we have performed several quantum chemistry studies to determine the pathways for proton transfer and chemical decomposition of these three prototypical salts.

15. SUBJECT TERMS Energetic Materials, High Energy Density Materials, Ionic Liquids, Strong Oxidizing Salts, Chemical Reactions, Melting, Proton Transfer

16. SECURITY CLASSIFICATION OF:

17. LIMITATION OF ABSTRACT

18. NUMBER OF PAGES

19a. NAME OF RESPONSIBLE PERSON

a. REPORT

b. ABSTRACT

c. THIS PAGE

10

19b. TELEPHONE NUMBER (include area code)

Final Technical Report
(AFOSR Grant No. F49620-00-1-0273)

**THEORETICAL STUDIES OF THE SENSITIVITY
OF ENERGETIC MATERIALS**

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Approved for Public Release
Distribution Unlimited

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Abstract

The research supported by AFOSR grant F49620-00-1-0273 for the period 15 April 2000 to 14 April 2003 is described. The purpose of this research program is to develop atomic-level models for high energy density materials (HEDM), and to study their fundamental properties and behaviors that determine their suitability as practical propellants and explosives. The central focus of our research during this grant period was ionic energetic materials, although some studies of the interactions and reactions of energetic molecules with solid Al and Al_2O_3 , and of the hydrogen-bonded energetic solid 1,1-diamino-2,2-dinitroethylene (FOX-7) were performed. The primary purpose of the work was to develop accurate models for describing the physical properties of strong oxidizing salts. We have successfully modeled crystal structures, melting, and liquid properties of ammonium dinitramide as a test case for our approaches, and we have partially developed models for ammonium nitrate and hydroxylammonium nitrate. A long-term goal of this work is to model the chemistry of ionic liquids and thus we have performed several quantum chemistry studies to determine the pathways for proton transfer and chemical decomposition of these three prototypical salts.

Technical Summary

The focus of this program was to develop a better understanding of and theoretical predictive capabilities for the fundamental physical and chemical properties of high energy density materials particularly strong oxidizing salts. The emphasis was on three kinds of energetic materials: (1) energetic salts, (2) hydrogen-bonded energetic materials, and (3) aluminum-energetic molecule composite materials. Most of the effort was devoted to (1), that is, ionic materials; however, significant progress was made for all three classes of materials. This research is motivated by the need for more energetic but less sensitive explosives and propellants. The predictive capabilities that are being developed in this project are important in the search for new energetic salts since experimentalists must invest considerable time and effort in determining the suitability of a proposed new salt as a practical energetic ionic liquid.

Physical Properties of Ionic Solids and Liquids

Our progress in developing accurate predictive theoretical capabilities for strong oxidizing salts is particularly significant. We achieved the proposed goal of developing and demonstrating theoretical methods for accurate simulations of the melting of complex energetic salts. We have shown that our methods predicts the exact solid-liquid transition as a function of pressure for ammonium dinitramide (ADN); that is, we reproduce, without empirical calibrations, the solid-liquid equilibrium curve over the range of chemical stability of the experimentally-determined pressure-temperature phase diagram.[1] More details of our studies of ADN are discussed below.

Although this result was the central focus of the work, the overall, long-term goal of our work on energetic ionic materials is much broader and comprehensive; that is, we are developing models to ultimately have the capability of simulating the chemical decomposition of energetic salts. We began this project with a plan of approach based on deliberative, step-by-step development of methods and models that accurately describe the basic structural and physical properties of various classes of novel energetic salts that are under consideration as replacements for ammonium perchlorate and for other applications (e.g., liquid ionic energetic materials). During the grant period we concentrated on ADN, ammonium nitrate (AN), and hydroxyl ammonium nitrate (HAN). We have now begun studies of 1-n-propyl-4-amino-1,2,4-triazole bromide. These particular salts were selected based on suggestions by researchers at AFRL, Edwards.

We began the work using plane-wave DFT and *ab initio* methods to develop intermolecular force fields that describe the various crystal phases of these salts. We computed various properties, including response to static pressure, by using these potentials in molecular dynamics simulations and showed that they yield predictions that are in good agreement with experimental data (e.g., X-Ray crystal structures, lattice energy, thermal expansion coefficients, etc).[2-4] The next step in the proposed plan of approach was to use these models to simulate melting, which we have completed for ADN,[5] thus demonstrating that we can accurately predict the melting point of a complex energetic salt. We are continuing studies of melting of salts to show that our approach is generally applicable. We have preliminary results for melting simulations of

AN and have begun studies of 1-n-propyl-4-amino-1,2,4-triazole bromide. The latter will serve to demonstrate our ability to predict important liquid-state properties of energetic salts. We are carrying out our investigations with close interactions with Dr. Greg Drake at AFRL, Edwards, who has performed experimental studies of this salt.

While the computed properties of liquid ADN are reasonable, it does not provide a critical test since few measurements of the liquid properties have been reported, due, no doubt, to the relatively short temperature range for which it is chemically stable. We computed the density, viscosity, and diffusion coefficient as functions of temperature for liquid ADN. Östmark and coworkers[6] report that the viscosity of ADN is "very low," but do not give a value for it. Our calculations give a value of the viscosity η that is indeed quite low compared to other ionic liquids. We computed the viscosity coefficient as a function of temperature at 1 atm. The results were fit by the function $\eta = Ae^{E_\eta/kT}$, with $A = 0.03939$ cp and $E_\eta/k = 608.5$ K. The measured density of ADN at 373 K from pycnometric measurements is 1.560 g/cm^3 . [6] Our calculated value is $1.58 \pm 0.01 \text{ g/cm}^3$, which is in excellent agreement with the measured value.

Our success in modeling melting of a complex salt such as ADN is not only of significance for practical interests, but it is also a major step forward in applications of molecular dynamics. Prior to our MD simulations of ADN melting, the most complicated salt for which melting had been simulated is NaCl (to our knowledge). We have shown that the melting is accurately described by a fixed-charge model and a standard type of force field. Thus, our results suggest that the methods can be readily generalized and easily transitioned for use by experimentalists who are exploring novel energetic ionic solids and liquids, which we are pursuing via interactions with Drs. Jerry Boatz and Greg Drake at AFRL, Edwards.

Chemical Reactions in Energetic Salts

Since a long-term goal of our work is to develop models to describe energetic salts under extreme conditions (shocking and heating) and undergoing chemical decomposition, we have begun studies of proton transfer and chemical reactions in the salts of interest in this program. Specifically we have used DFT and *ab initio* methods to determine the reaction pathways in isolated ion pairs and acid-base pairs (the nature of the pair depends on whether proton transfer occurs) and in clusters of these pairs. Sublimation or evaporation of ammonium salts involve the conversion of ion pairs (which are the components in the solids and liquids) to acid-base pairs by transfer of a proton from the cation to anion. By determining the equilibrium and transition state structures of successively larger clusters of ion/acid-base pairs, we attempt to approach the properties of the bulk. In doing this we take advantage of what has been learned by very extensive studies of the similar process of the hydration of acids. These properties of proton transfer in clusters can be used to develop models that apply to all phases, – solids, liquids, and gases – and the transitions between them.

The following are brief descriptions of the results of our studies of proton transfer in these ionic systems.

Ammonium Nitrate. Proton transfer in ammonia-nitric acid clusters containing up to four acid-base pairs were studied by using DFT and MP2 (second-order Möller-

Plesset) methods.[7] We also studied AN solvated by a single ammonia or a single nitric acid molecule. Proton transfer does not occur in a single AN, although the ammonia is strongly hydrogen bonded to the nitrate: $\text{H}_3\text{N}\cdots\text{HNO}_3$. Proton transfer does occur in dimers and larger clusters of AN, and the resulting ions are bound by ionic forces. Solvation of a single AN by HNO_3 results in proton transfer in the AN, however, no proton transfer occurs upon solvation by an ammonia molecule.

The main determinant for proton transfer appears to be the magnitude of the electrostatic energy between the components of the clusters. Although the absolute value of the electrostatic energy depends on the way in which charge is partitioned among the atoms, relative values of this energy in various clusters can be used to determine whether or not proton transfer will occur. Previously, the binding energy per molecular unit in a cluster was taken to be an indication of the ionic bonding; however, we find that the binding energy alone does not give an unambiguous indication of ionic interactions and proton transfer.

Ammonium Dinitramide. The structures, energies and vibrational frequencies of ammonium dinitramide, $[\text{ADN}]\text{NH}_3$, $[\text{ADN}]\text{HDN}$, and $[\text{ADN}]_2$ were calculated by using DFT.[8] Whereas a single ADN molecule is stabilized by hydrogen bonding, the complexes $[\text{ADN}]\text{NH}_3$, $[\text{ADN}]\text{HDN}$, and $[\text{ADN}]_2$ are ionic as a result of a proton transfer from HDN to NH_3 . It is reasonable to assume that larger clusters are ionic as well. Proton transfer in the complexes is accompanied by notable structural changes in the dinitramide group. The $-\text{NO}_2$ groups in ADN are initially in an eclipsed like configuration, giving the molecule a symmetry plane. Upon proton transfer, the NO_2 groups undergo torsional motion to become staggered. These structural rearrangements facilitate the formation of the transition state for $\text{H}_3\text{N}-\text{N}-\text{N}(\text{NO}_2)_2 \rightarrow \text{NH}_4\text{NO}_3 + \text{N}_2\text{O}$ and affect the rate of ADN chemical decomposition.

The magnitude of the electrostatic energy between the different components of the cluster that was established as a criterium for proton transfer in our study of ammonium nitrate clusters, which we discussed above, is also seen to be valid in the present case. For example, whereas the binding energy of the ADN unit is about 30% smaller than that of the $[\text{ADN}]\text{NH}_3$ complex (13.6 compared to 19.7 kcal/mol), the low values of $E(\text{coulombic})$ in ADN (-5.5 kcal/mol), compared to $[\text{ADN}]\text{NH}_3$ (-63 kcal/mol), however, gives a specific indication that proton transfer has not occurred.

Many of the same aspects of proton transfer in ammonium nitrate clusters also apply to ammonium dinitramide clusters. In both cases, the acid components HNO_3 and $\text{HN}(\text{NO}_2)_2$ are not strong enough to introduce proton transfer in a single monomer unit, and the electrostatic interactions between an anion and cation pair do not provide sufficient stabilization energy to compensate for breaking the covalent bond of the acidic proton. The presence of solvating groups increases the electrostatic interaction energy in the cluster and proton transfer occurs. Large structural changes accompany the proton transfer process and the vibrational frequencies of the hydrogen bonded NH bonds undergo large shifts.

Hydroxylammonium Nitrate. Structures and energies of gas-phase hydroxylammonium nitrate (HAN), HONH_3NO_3 , were calculated by using DFT with a 6-311++G(*d,p*) basis set.[9] Three stable configurations were found for HAN, which involve strong hydrogen bonding between the hydroxylamine and nitric acid molecules. In the most stable configuration, both the oxygen and the nitrogen of hydroxylamine are

hydrogen bonded to sites on the nitric acid molecule. In the less stable HAN structures only the oxygen or the nitrogen of hydroxylamine are hydrogen-bonded. Two stable structures for the (HAN)₂ complex were investigated. The more stable structure is ionic, with the nitric acid proton having been transferred to the nitrogen of hydroxylamine. Strong electrostatic and hydrogen-bonding interactions stabilize this structure. The other stable form of (HAN)₂ has fewer hydrogen bonds and is composed of interacting neutral nitric acid and hydroxylamine molecules. Binding energies were determined for all structures along with corrections for basis set superposition errors in the HAN molecules. Proton exchange reaction paths were investigated. The saddle points for the proton exchange are ionic forms of HAN with interacting HONH₃⁺ and NO₃⁻ moieties. These ionic structures are 13.5 and 13.6 kcal/mol higher in energy than the neutral hydrogen-bonded complexes of HONH₂ and HNO₃ from which they are formed. The electrostatic attraction between the ions is sufficient to stabilize the ionic form of (HAN)₂, whereas in the HAN monomer the interaction energy for single HONH₃⁺ and NO₃⁻ ions is not sufficient to compensate for the energy required for proton transfer from nitric acid to the hydroxylamine group.

Chemical Decomposition of Gas-Phase Ammonium Dinitramide. The chemical decomposition of ionic liquids presents a more challenging problem. We have performed some calculations during this grant period that provides the basis for developing realistic models that describe the initial decomposition reactions. However, much remains to be done to develop these models.

Our initial study focused on the decomposition reactions in ammonium dinitramide and represents the first stage in the development of a model for the chemistry that occurs in the various phases under various conditions. More specifically, we performed quantum chemistry calculations to determine the various decomposition pathways in the acid that is the result of sublimation or evaporation of ammonium dinitramide, i.e., dinitramic acid.[10] Gas-phase dinitramic acid HN(NO₂)₂ [HDN] decomposes along two pathways, one involving a molecular rearrangement, HDN → HNO₃ + N₂O, and a second initiated by N-N bond fission, HDN → H \dot{N} NO₂ + \dot{N} O₂. A molecular rearrangement pathway for the gas phase dinitramide ion N(NO₂)₂⁻ DN⁻ → NO₃⁻ + N₂O, can also occur. The rates and pathways for the decomposition of HDN and the corresponding dinitramide ion are subjects of the present work. Density functional theory calculations at the B3LYP/6-311G(d,p) level were carried out to determine the geometries, vibrational frequencies, and zero-point energies of the reactants, products, and transition states involved in the gas phase decomposition of HDN. These geometries were used in the Modified Gaussian-2 method (G2M) to calculate energies to sufficient accuracy to predict the rates of the decomposition reactions. The lowest energy pathway for N₂O formation initially involves an internal proton transfer in the HDN molecule. The system then passes through a four-center transition state that has a protonated bridge oxygen atom. The energy of this geometry is 35.2 kcal/mol higher than the reactant from which it is formed. This pathway has not been previously identified. The rates of the N₂O elimination pathways were calculated using the RRKM theory. The rates of HDN and DN⁻ decomposition are compared to each other and to the rate of N-N bond fission in dinitramic acid.

Adsorption and Decomposition of Nitromethane and FOX-7 Molecules on the Al(111) Surface

First-principles calculations based on spin unrestricted DFT and the generalized gradient approximation were used to study the adsorption of nitromethane and 1,1-diamino-2,2-dinitroethylene (FOX-7) molecules on the Al(111) surface.[11] The calculations employed (3×3) aluminum slab geometries and 3D periodic boundary conditions. The calculations show that both dissociative and nondissociative adsorption occurs, depending on the molecular orientation and the particular surface sites involved. In the case of dissociative chemisorption, O-atom abstraction by Al surface atoms is the dominant mechanism. The dissociated oxygen atom forms strong Al—O bonds with the neighboring Al sites around the dissociation sites. Additionally, the radical species obtained as a result of oxygen atom elimination remains bonded to the surface. In some instances, both oxygen atoms of the nitro group dissociate and oxidize the aluminum surface. Finally, for the case of nondissociative adsorption, various N-O-Al bridge-type bonding configurations can be formed. Based on the data provided from these studies it can be concluded that oxidation of the aluminum surface readily occurs, either by partial or complete dissociation of the oxygen atoms from the NO₂ group.

Studies of Gas-Phase and Crystalline 1,1-diamino-2,2-dinitroethylene (FOX-7)

Ab initio molecular orbital and plane-wave methods were used to calculate the structural and vibrational properties of 1,1-diamino-2,2-dinitroethylene (FOX-7). This is a highly efficient, low sensitivity explosive that has yet to be put to practical use, however, it serves as an excellent example of hydrogen-bonded high energy density material (HEDM) and thus is being widely studied. The calculated gas-phase structures agree well with the experimental X-ray data except the nitro and amino groups are larger than those observed in the solid. The IR spectra were computed for the three isomers of FOX-7, i.e., the 1,1; 1,2-*cis*; and 1,2-*trans* isomers. The order of stability of these isomers is predicted to be: 1,1; 1,2-*trans*; and 1,2-*cis*. The structural properties of crystalline FOX-7 were studied by using a plane-wave DFT method. Periodic boundary conditions in all three directions were used. The structure was optimized with full relaxation of the atomic positions and the lattice parameters under P2₁/*n* symmetry. The calculated structure is in good agreement with the X-ray structure.

We also developed an intermolecular potential to describe solid FOX-7 assuming rigid molecules. We performed crystal-packing calculations that demonstrate that this potential accurately predicts the correct crystallographic features and lattice energy. Isothermal-isobaric MD simulations using this potential were carried out at atmospheric pressure over the temperature range 4.2-450 K. These calculations show that increasing temperature has little effect on the molecular orientations within the unit cell. The computed thermal expansion coefficients show anisotropic behavior of the solid with the largest expansion being along the *b* crystallographic direction.

This model accurately describes solid FOX-7. It is relatively straightforward to extend the model to include intramolecular forces such that it can be used to study various properties such as energy transfer (e.g., in response to shocking) and melting.

Further modifications could be made to incorporate initial chemical changes in condensed-phase FOX-7.

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10. S. Alavi and D. L. Thompson, "Rates and Mechanism of the Gas-Phase Decomposition of Ammonium Dinitramine," *J. Chem. Phys.*, in press.
11. D. C. Sorescu, J. A. Boatz, and D. L. Thompson, *J. Phys. Chem. A* **105**, 5010 (2001).

Accomplishments/New Findings:

- We have developed atomic-level models that accurately describe the solid states of ammonium nitrate and ammonium dinitramide.
- We have developed an atomic-level model that accurately describes hydrogen-bonded crystalline FOX-7 (1,1-Diamino-2,2-Dinitroethylene).
- We have demonstrated that our method accurately predicts the melting point of ammonium dinitramide.
- We have used DFT calculations to determine the proton transfer pathways and energetics for clusters of ammonium nitrate, ammonium dinitramide, and hydroxylammonium nitrate.
- We have used DFT calculations to determine the pathways and energetics for the chemical decomposition of gas-phase ammonium dinitramide.
- We have used plane-wave DFT methods to investigate the chemical decomposition of nitromethane and FOX-7 on solid aluminum.

Personnel Supported:

Professor Donald L. Thompson, Principal Investigator (2 summer months)
Dr. Dan C. Sorescu, Postdoctoral Research Associate (half-time for 4 months)
Dr. Saman Alavi, Postdoctoral Research Associate (partial support).
Dr. Gustavo F. Velardez, Postdoctoral Research Associate (partial support).

Publications

1. Dan C. Sorescu and Donald L. Thompson, "*Classical and Quantum Mechanical Studies of Crystalline Ammonium Nitrate*," J. Phys. Chem. A **105**, 720-733 (2001).
2. Dan C. Sorescu, Jerry A. Boatz, and Donald L. Thompson, "*Classical and Quantum Mechanical Studies of Crystalline FOX-7 (1,1-Diamino-2,2-Dinitroethylene)*," J. Phys. Chem. A **105**, 5010-5021 (2001).
3. Dan C. Sorescu and Donald L. Thompson, "*Quantum Mechanical Studies of Pressure Effects in Crystalline Ammonium Dinitramide*," J. Phys. Chem. A **105**, 7413-7422 (2001).
4. Saman Alavi and Donald L. Thompson, "*Theoretical Study of Proton Transfer in Ammonium Nitrate Clusters*," J. Chem. Phys. **117**, 2599-2608 (2002).
5. Saman Alavi, Dan C. Sorescu, and Donald L. Thompson, "*Adsorption of HCl on a Single-Crystal α -Al₂O₃ (0001) Surface*," J. Phys. Chem. B **107**, 186-195 (2003).
6. Saman Alavi and Donald L. Thompson, "*Proton Transfer in Ammonium Dinitramide Clusters*," J. Chem. Phys. **118**, 2599-2605 (2003).
7. Saman Alavi and Donald L. Thompson, "*Rates and Mechanism of the Gas-Phase Decomposition of Ammonium Dinitramine*," J. Chem. Phys., in press.
8. Saman Alavi and Donald L. Thompson, "*Hydrogen Bonding and Proton Transfer in Small Hydroxylammonium Nitrate Clusters. A Theoretical Study*," J. Chem. Phys., in press.
9. Dan C. Sorescu, Jerry A. Boatz, and Donald L. Thompson, "*First-Principles Calculations of the Adsorption of Nitromethane and 1,1-Diamino-2,2-dinitroethylene (FOX-7) Molecules on the Al(111) surface*," J. Phys. Chem., in press.
10. Gustavo Velardez, Saman Alavi, and Donald L. Thompson, "*Molecular Dynamics Study of Melting and Liquid Properties of Ammonium Dinitramide*," J. Chem. Phys., in press.
11. Dan C. Sorescu, Jerry A. Boatz, and Donald L. Thompson, "*First-Principles Calculations of the Interactions of Nitromethane and 1,1-Diamino-2,2-dinitroethylene (FOX-7) Molecules with solid Al₂O₃*," Manuscript in preparation.

Interactions/Transitions:

Oral presentations of the results of the work:

- Energetic Materials Gordon Conference, Tilden, N. H.; July 2-7, 2000.
- 2000 High Energy Density Matter Contractor's Meeting, Park City, UT; October 24-26, 2000.
- Distinguished Alumni Lecture, Department of Chemistry, University of Arkansas, Fayetteville; April 14, 2003

The following **collaborations** were established:

- Collaborations with Dr. Jerry Boatz (AFRL, Edwards), aided by support from a Multiscale Simulations of HEDM Challenge Project, is ongoing. The work is focused on chemical reactions occurring on Al and Al₂O₃ solids and on simulations of melting of ionic solids and calculations of the liquid-state properties.
- A collaboration with Mark Gordon (Iowa State University) to develop realistic models for simulating ionic liquids by using the Effective Fragment Potential (EFP) approach.
- Interactions with Dr. Greg Drake (AFRL, Edwards) to transition our methods for simulating melting and predicting liquid properties of energetic salts for practical applications.
- Participated in a HPC Challenge grant project with Dr. Jerry Boatz (AFRL, Edwards).

New discoveries, inventions, or patent disclosures

None

Honors/Awards

None